

ABSTRACT

A binding site in nuclear hormone receptors is described and its structural coordinates [REDACTED] are provided. The invention provides machine-readable data storage media comprising structure coordinates of Site II and computer systems comprising 5 the machine-readable data storage media. The invention provides methods used in the design and identification of ligands of Site II and of modulators of nuclear hormone receptors. The invention provides ligands of Site II, modulators of NHRs, pharmaceutical compositions comprising modulators of NHRs, methods of modulating NHRs, and methods of treating diseases by administering modulators of 10 an NHR. Also provided are methods of designing mutants, mutant NHRs, Site II binding assays, and models of Site II.